A Multiscale Meshfree Method for the Mechanical Analysis of Low Dimensional Nanostructures

Dong Qian* and Wing Kam Liu**

*University of Cincinnati, Cincinnati, OH 45221-0072, USA, Dong.Qian@uc.edu
**Northwestern University, Evanston, IL 60208-0031, USA, w-liu@northwestern.edu

ABSTRACT

A multiscale meshfree approach for the mechanical analysis of low dimensional nanostructures is proposed, with the objective that both computational efficiency and accuracy can be achieved for systems involving large number of atoms or molecules. This method is implemented through a so-called "bridging scale" term, which is constructed by projecting the molecular dynamics (MD) solution onto its coarse scale approximation. The multiscale decomposition is obtained by subtracting the bridging scale component from the MD solutions. With this decomposition and a physics-based atomic potential, the coupled nonlinear governing equations between the coarse and fine scales are derived and solved using Newton's method. The advantages of the method can be briefly summarized as follows: First of all, the multiscale projection effectively decouples the incremental form of the multiscale equations. In addition, the coarse scale and fine scale treatments are unified in one formulation, in particular, the classical hyperelastic stress (sometimes involves higher order stress) update scheme is replaced with a simpler treatment at the atomic level in the coarse scale part of the method. Meshfree approximations are introduced for interpolating the low dimensional nano-structures. Particular advantage of this approach is that the approximation automatically satisfies the high order continuity requirement, which is essential for properly representing curved surfaces and lines at nanoscale. Finally, Comparisons with MD on bending of carbon nanotubes are made. Good agreement on the buckling pattern and energy shows the robustness of the method.

Keywords: Meshfree method, multiscale method, nanomechanics, nanostructures, carbon nanotubes.

1 INTRODUCTION

Tremendous amount of progress has been made in the past decade in the field of synthesis of new low-dimensional nanostructures. Examples of such include nano-particles, nano-fibers and nano-platelets. The low-dimensionality, when combined with their exceptional physical properties such as high strength, stiffness, low mass density and almost defects-free structure, make it ideal for them to be used as reinforcing materials in high strength, light weight composites, as component of integrated nano-electro-mechanical systems (NEMS), and as part in other technological applications. For instance, carbon nanotube (CNT) which was discovered by Iijima [1] in 1991 has found applications in field emission displays [2, 3] and composites [4]. To achieve the understanding of the mechanical behaviors of these systems in which CNTs are integrated with devices or structures that are larger in length scale, a hierarchical modeling approach that accounts for the effect of different length scales must be taken. Single scale methods such as molecular dynamics (MD) or finite element methods (FEM) will have difficulties in terms of either computational efficiency or accuracy. For instance, CNTs are typically a few hundreds of nano-meters in length and can contain millions of atoms. Performing a full-scale MD simulation in this case is a great challenge. In addition, the mechanical response of the CNT measured in experiment is typically on the order of second, in contrast the time steps in MD is restricted to several pico-second. These gaps highlight the need for multiscale methods that aim at combining the strength of computational methods at both atomic and continuum scale.

In this paper a multiscale method based on the concept of "bridging scale" is developed. This concept was originally proposed by Liu et al [5] and has been successfully applied in problems involving strain localization [6], boundary layers [7] and coupling of finite elements with meshfree shape functions [8]. In this paper, we will focus on zero temperature problems and dynamic effects are not considered. A multiscale framework for finite temperature problem has recently been proposed by Wagner and Liu [9].

In order to accurately describe the geometry at nanoscale, meshfree approximation is introduced. Correspondingly the solution based on the meshfree shape functions is referred to as the coarse scale part of the solution. The fine scale solution is simply interpreted as the part that can not be represented by the solution based on meshfree shape function. The full-scale MD equation is needed in order to obtain the fine scale part of the solution. Note that it is not necessary to perform full-scale MD in the entire domain as long as the coarse scale representation is valid for most of the region. Full-scale MD is only used in the regions where the deformation becomes local and the detailed atomic structure has to be accurately accounted for. One typical example is the development of dislocation.

To ensure the consistency between the fine scale solution from MD and the coarse scale solution, a bridging scale projection is defined. The effect of this projection is that it decouples the internal force in the incremental form of the governing equation. Compared with a typical mesh refinement or "handshake model", the major difference is that here the coarse scale solution exists in the entire domain, and molecular structure is added on top of the meshfree discretization in the enrichment region. The details of the multiscale method and implementation will be outlined in the next section. Examples of applying this method to nanotube structures are presented in section 3. Final conclusion and discussion on further extension of the method are given in section 4.

2 MULTISCALE GOVERNING EQUATION AND SOLUTION PROCEDURE

2.1 The Bridging Scale Projection

Before introducing any specific solution procedure, we first partition the total scale variables into two scales as follows

$$\boldsymbol{u} = \bar{\boldsymbol{u}} + \tilde{\boldsymbol{u}} \tag{1}$$

in which "-" denotes the coarse scale and "~" represents the fine scale.

Define a coarse scale projection operator such that $\bar{\boldsymbol{u}} = \boldsymbol{P}\bar{\boldsymbol{u}}$ and apply $\boldsymbol{P}$ to both side of Eq.(1), we have

$$\bar{\boldsymbol{u}} = \boldsymbol{P}\bar{\boldsymbol{u}} = \boldsymbol{P}\left(\boldsymbol{u} - \tilde{\boldsymbol{u}}\right) \tag{2}$$

Substitute this back to Eq,(1) gives

$$\boldsymbol{u} = \boldsymbol{P}\boldsymbol{u} + \tilde{\boldsymbol{u}} - \boldsymbol{P}\tilde{\boldsymbol{u}} \tag{3}$$

In Eq.(3), $\boldsymbol{P}\tilde{\boldsymbol{u}}$ is the bridging scale term that we have been referring to in the introduction section. It effectively cancels any overlapping components between $\bar{\boldsymbol{u}}$ and $\tilde{\boldsymbol{u}}$.

$\boldsymbol{P}\boldsymbol{u}$ in Eq.(3) can be represented by a set of particles and associated shape functions, i.e.,

$$\bar{\boldsymbol{u}}\left(X_\alpha\right) = \sum_I N_I\left(X_\alpha\right)\boldsymbol{d}_I \tag{4}$$

in which capital letters in the subscripts are the indices for nodes and Greek letters are for atoms. A simple direct notation corresponding to (4) is

$$\bar{\boldsymbol{u}} = \boldsymbol{N}\boldsymbol{d} \tag{5}$$

$\boldsymbol{N}$ in Eq.(5) is the shape function matrix (not necessary a square matrix) that relates the nodal displacement to the atomic displacements. Note that the $\boldsymbol{d}$ is not simply solved from the single scale finite element method because of the coupling between the coarse and fine scales.

A seemingly natural way of obtaining $\boldsymbol{P}\tilde{\boldsymbol{u}}$ is to solve the equation

$$\boldsymbol{N}\boldsymbol{v} = \tilde{\boldsymbol{u}} \tag{6}$$

in which $\boldsymbol{v}$ is the variable that is defined at the node. However, the fact that $\boldsymbol{N}$ is not always a square matrix makes it impossible to get the solution to $\boldsymbol{v}$ based on Eq.(6). An alternative is to minimize the difference between $\boldsymbol{N}\boldsymbol{v}$ and $\tilde{\boldsymbol{u}}$ based on certain measure. One way is to obtain $\boldsymbol{v}$ by minimizing the following term

$$e = \left(\tilde{\boldsymbol{u}} - \boldsymbol{N}\boldsymbol{v}\right)^T \boldsymbol{k}_v \left(\tilde{\boldsymbol{u}} - \boldsymbol{N}\boldsymbol{v}\right) \tag{7}$$

in which $\boldsymbol{k}_v$ is a general symmetric kernel matrix. In the case that dynamic effects are not considered, we can define $\boldsymbol{k}_v$ as the tangent stiffness matrix corresponding to a specific iteration step v. This matrix is needed as part of the Newton's method to be described in the next section. Given the fact that $\boldsymbol{k}_v$ can be decomposed into the product of an upper and lower triangular matrix, i.e., $\boldsymbol{k}_v = \boldsymbol{L}_v^T \boldsymbol{L}_v$, minimizing Eq.(7) gives

$$\boldsymbol{v} = \left(\boldsymbol{N}_L^T \boldsymbol{N}_L\right)^{-1} \boldsymbol{N}_L^T \tilde{\boldsymbol{u}}_L \tag{8}$$

in which $\tilde{\boldsymbol{u}}_L = \boldsymbol{L}_v \tilde{\boldsymbol{u}}$ and $\boldsymbol{N}_L = \boldsymbol{L}_v \boldsymbol{N}$

Therefore from $\boldsymbol{P}\tilde{\boldsymbol{u}} = \boldsymbol{N}\boldsymbol{v}$, we get the definition of the coarse scale projection operator, i.e.,

$$\boldsymbol{P} = \boldsymbol{N}\left(\boldsymbol{N}_L^T \boldsymbol{N}_L\right)^{-1} \boldsymbol{N}_L^T \boldsymbol{L} \tag{9}$$

Define $\boldsymbol{Q}=\boldsymbol{I}-\boldsymbol{P}$, the multilscale decomposition can then be expressed as

$$\boldsymbol{u} = \bar{\boldsymbol{u}} + \tilde{\boldsymbol{u}} = \boldsymbol{N}\boldsymbol{d} + \boldsymbol{Q}\tilde{\boldsymbol{u}} \tag{10}$$

2.2 Governing Equations and solution procedures

Based on the principle of virtual work, we have

$$\delta W(\boldsymbol{u}) = \frac{\partial W}{\partial \boldsymbol{u}} \delta \boldsymbol{u} = \frac{\partial W}{\partial \boldsymbol{u}} \left(\boldsymbol{N} \delta \boldsymbol{d} + \boldsymbol{Q} \delta \tilde{\boldsymbol{u}} \right) = 0 \quad (11)$$

which can be further expressed into the following two equations

$$\boldsymbol{N}^T \boldsymbol{f}^{int}(\boldsymbol{d}, \tilde{\boldsymbol{u}}) = \boldsymbol{N}^T \boldsymbol{f}^{ext}(\boldsymbol{d}, \tilde{\boldsymbol{u}}) \quad (12a)$$

$$\boldsymbol{Q}^T \boldsymbol{f}^{int}(\boldsymbol{d}, \tilde{\boldsymbol{u}}) = \boldsymbol{Q}^T \boldsymbol{f}^{ext}(\boldsymbol{d}, \tilde{\boldsymbol{u}}) \quad (12b)$$

Due to the nonlineaity of the inter-atomic potential, we introduce Newton's method to solve for Eqs (12a) and (12b). The incremental form of the governing equation corresponding to Eqs. (12) is

$$\begin{bmatrix} \boldsymbol{N}^T \boldsymbol{k}_v \boldsymbol{N} & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{Q}^T \boldsymbol{k}_v \boldsymbol{Q} \end{bmatrix} \begin{Bmatrix} \Delta \boldsymbol{d} \\ \Delta \tilde{\boldsymbol{u}} \end{Bmatrix} = \begin{Bmatrix} \boldsymbol{N}^T \boldsymbol{f}^{ext} - \boldsymbol{N}^T \boldsymbol{f}^{int}(\boldsymbol{d}_v, \tilde{\boldsymbol{u}}_v) \\ \boldsymbol{Q}^T \boldsymbol{f}^{ext} - \boldsymbol{Q}^T \boldsymbol{f}^{int}(\boldsymbol{d}_v, \tilde{\boldsymbol{u}}_v) \end{Bmatrix} \quad (13)$$

Note that the off-diagonal terms vanish due to the properties of the projection that have been defined. It is also trivial to verify that $\boldsymbol{N}^T \boldsymbol{k}_v \boldsymbol{Q} = \boldsymbol{0}$. The second row of the matrix in Eq.(13) can be replaced by the molecular dynamics equation due to the fact the $\boldsymbol{Q}$ is a singular matrix. In the numerical implementation, the secant stiffness is used as an approximation for the tangent stiffness, which provides substantial computational saving when combined with a non-linear conjugate gradient method.

A method of introducing scalability to the solution procedure for Eq. (13) is recently proposed by Qian et al [10]. This approach is valid for treating both bonded and non-bonded interactions in the system. In this method, the energy is distributed to the surfaces or the lines of the low dimensional nanomaterials. One can then substitute the exact summation on the atoms as implied in Eq.(13) with an equivalent summation on the quadrature points. As a result, there is no need to derive a hyper-elastic type of stress update scheme. This is particularly efficient for complex lattices.

3 MESHFREE APPROXIMATION

Meshfree method is a new generation method that was developed in recent decades. A comprehensive review of the subject can be found in please see [11] and two pecial journal issues [12, 13] that have been devoted to this topic.

As a moving least square type of interpolation, the advantage of using this technique is that the geometric factors such as bond length, bonding angle can be accurately captured by the approximation. These factors are common variables in evaluating the binding energy of a particular molecular system. However, one of the difficulties is that simply prescribing particles along a line or on a 2-D surface is going to violate the admissible condition. We propose an iso-parametric type of meshfree method. We define three different configurations, the iso-parametric configuration, the undeformed configuration and the deformed configuration. The meshfree shape functions are defined in the iso-parametric domain. Both the geometries in the undeformed and deformed configurations are established using this shape function. Due to the fact that we are dealing with low-dimensional structures in a 3D space, the shape function is defined in 2D for a surface and 1D for a line. This is much more efficient when compared with a typical 3D formulation.

4 EXAMPLES

The system to be studied is a (10,10) carbon nanotube consists of 1900 atoms. The length of the tube is 11.56 nm. Bending angles are imposed at both ends of the tube at an incremental step of 0.25 degree. This corresponds to 0.5 degree for each step for a total of 30 steps. In the multicale method, the original system is now replaced with 380 particles. In addition, a nanotube structure consists of 17 hexagons is added as enrichment in order to capture the detail of the buckling mode. Shown in Figure 1 is an illustration of the enrichment scheme.

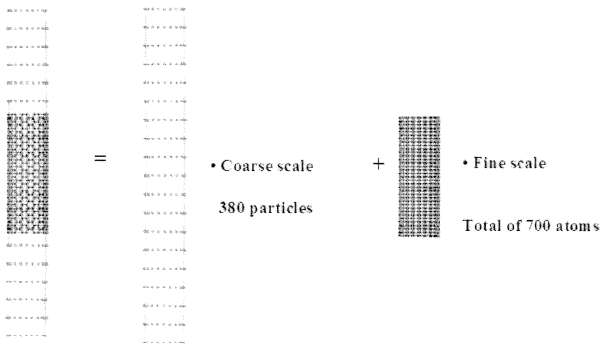

Figure 1: Multiscale analysis of bending of (10,10) CNT.

The accuracy of the method can be evaluated by comparing the results with those from a full-scale MD. Shown in Figure 2 are the final buckling patterns from the multiscale method and MD, it can be seen that the deformations from two different methods match well. In addition, the comparison in terms of the bending energy is shown in Figure 3 and it is found that the errors are no more than 1% for all the bending angles.

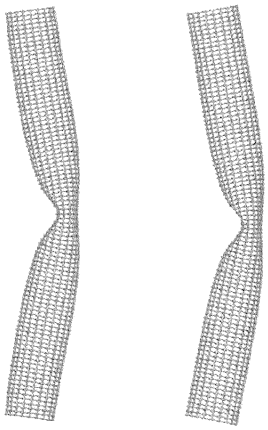

Figure 2: Comparison of buckling patterns for a (10,10) carbon nanotube (left) from proposed method. (right) from full-scale MD.

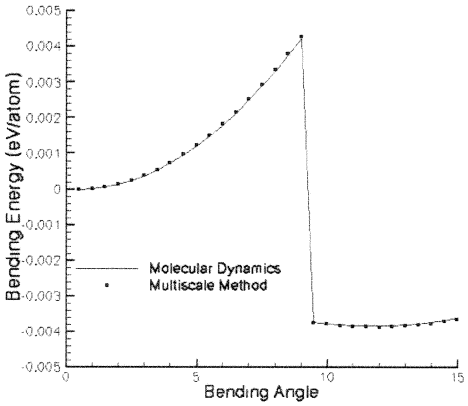

Figure 3: Comparison of bending energy.

5 CONCLUSION

Based on the concept of bridging scale, a multiscale projection method for the analysis of low-dimensional nano-structure is proposed. The method links a physics-based interatomic interaction to the mechanical properties of a low-dimensional nanoscale molecule. Meshfree shape functions are introduced to approximate the nanoscale lines and surfaces. A bendmark problem on carbon nanotube is presented to illustrate the robustness of the method. The method presented can be applied to a general class of application involving low-dimensional nanoscale materials.

6 ACKNOWLEDGEMENT

The support of this work to QD from the Ohio Board of Regents is gratefully acknowledged.

References

1. Iijima, S., *Helical Microtubules of Graphitic Carbon.* Nature. **354**(6348): p. 56-58,1991.
2. Normile, D., *Technology - Nanotubes generate full-color displays.* Science. **286**(5447): p. 2056-2057,1999.
3. Choi, W.B., et al., *Fully sealed, high-brightness carbon-nanotube field-emission display.* Applied Physics Letters. **75**(20): p. 3129-3131,1999.
4. Qian, D., et al., *Load transfer and deformation mechanisms in carbon nanotube- polystyrene composites.* Applied Physics Letters. **76**(20): p. 2868-2870,2000.
5. Liu, W.K., R.A. Uras, and Y. Chen, *Enrichment of the finite element method with the reproducing kernel particle method.* Journal of Applied Mechanics-Transactions of the Asme. **64**(4): p. 861-870,1997.
6. Hao, S., W.K. Liu, and D. Qian, *Localization-induced band and cohesive model.* Journal of Applied Mechanics-Transactions of the Asme. **67**(4): p. 803-812,2000.
7. Wagner, G.J., et al., *The extended finite element method for rigid particles in Stokes flow.* International Journal for Numerical Methods in Engineering. **51**(3): p. 293-313,2001.
8. Wagner, G.J. and W.K. Liu, *Hierarchical enrichment for bridging scales and mesh-free boundary conditions.* International Journal for Numerical Methods in Engineering. **50**(3): p. 507-524,2001.
9. Wagner, G.J. and W.K. Liu, *Coupling of atomistic and continuum simulations using a bridging scale decomposition(submitted).* Journal of Computational Physics,2002.
10. Qian, D., G.J. Wagner, and W.K. Liu, *A multiscale projection method for the analysis of carbon nanotubes (submitted).* Computer method in applied mechanics and engineering,2002.
11. Li., S.F. and W.K. Liu, *Meshfree and particle methods.* Applied Mechanics Reviews. **55**(1): p. 1-34,2002.
12. Liu WK Belytshko T and Oden JT, *Computer Methods in Applied Mechanics and Engineering.* Vol. 139, Amsterdam: North-Holland Pub. Co.,1996.
13. Chen JS and Liu WK (eds), *Computational Mechanics*. Vol. 25: Springer-Verlag,2000.